

# Searching for Complex Organic Molecules in Space

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This project funded by:  
NASA Science Mission Directorate Applied Information Research  
Program (AISR): 05-AISR05-0143 (Knuth PI, Carbon co-I)

# Orion



Photo Credit: Matthew Spinelli

# Orion Nebula



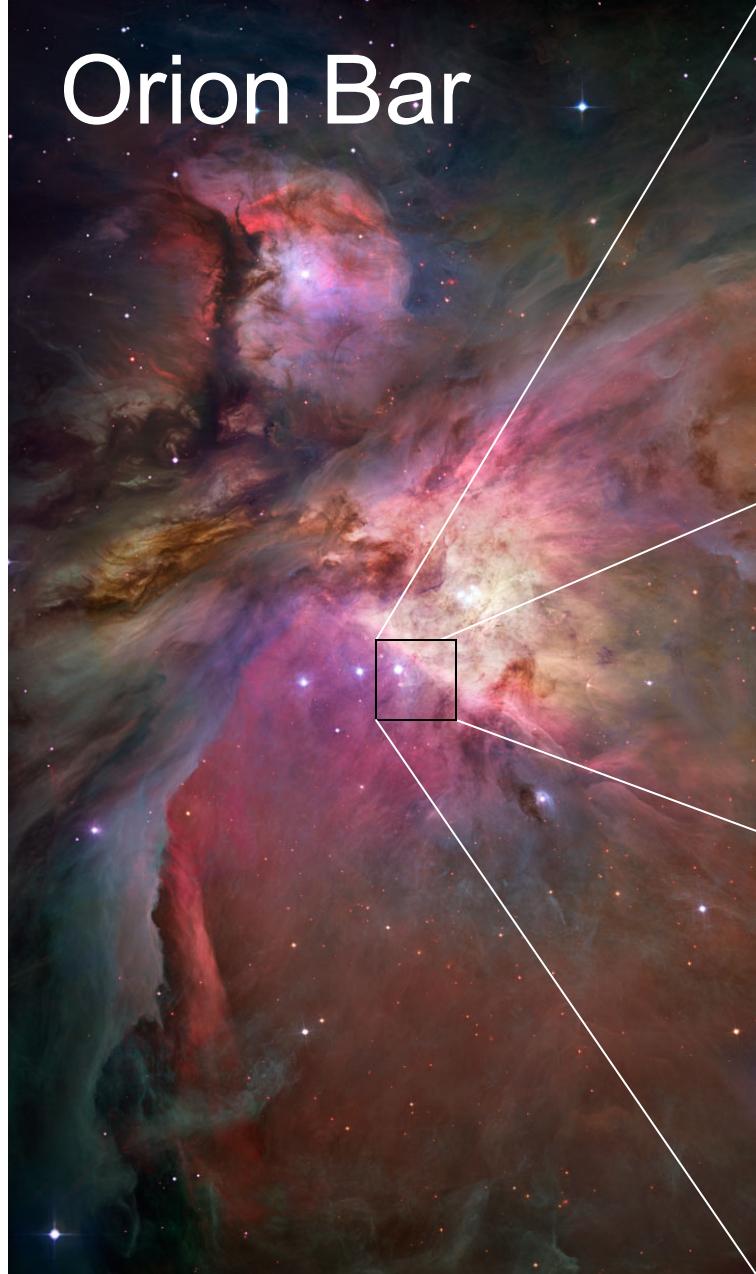
HST

5 May 2008

NASA AISRP PI Meeting

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# Orion Bar



5 May 2008

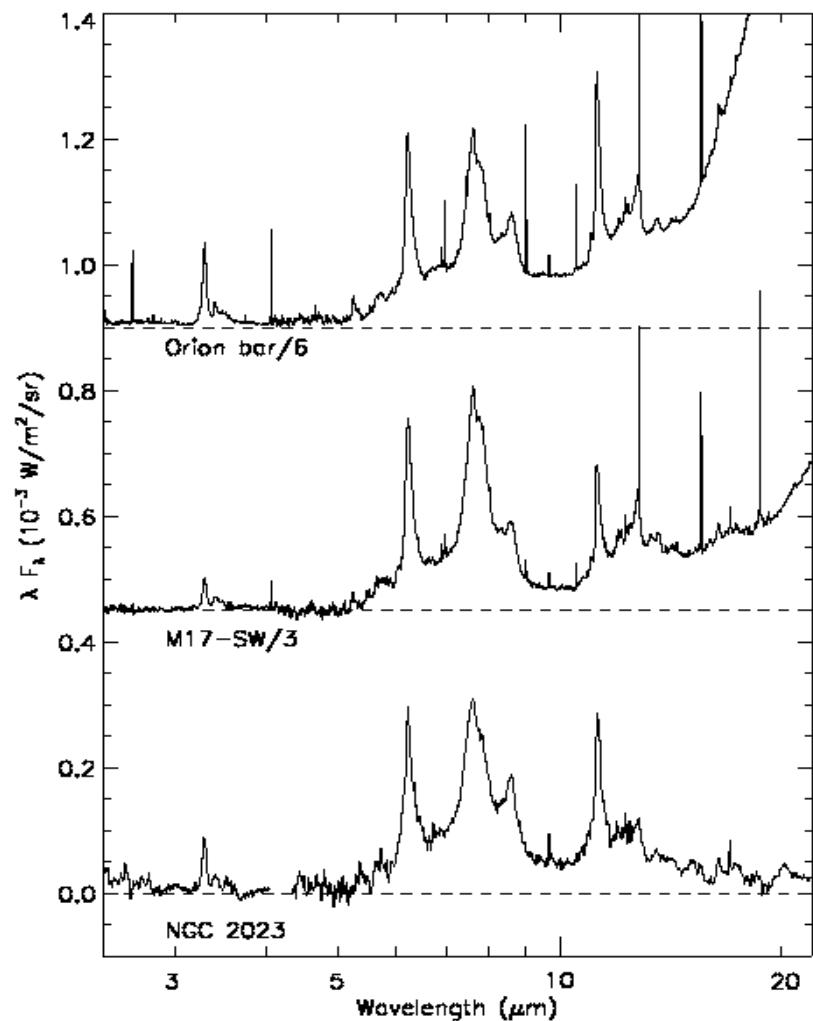


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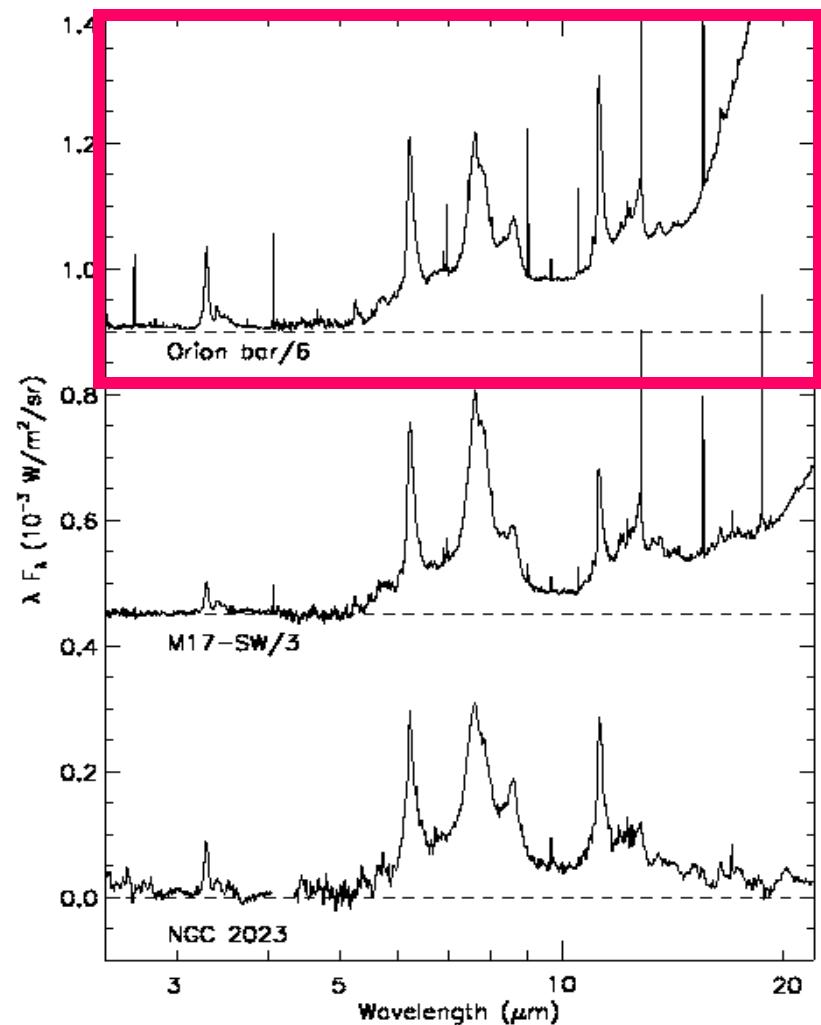
# Unidentified InfraRed (UIR) Emission

- UIR emission when there is UV-lit dust
- emission **near** 3.3, 6.2, 7.7, 8.6 and 11.2  $\mu\text{m}$ .
- dying stars, forming stars/planetary systems, ISM
- other galaxies,  $z = 2.8$



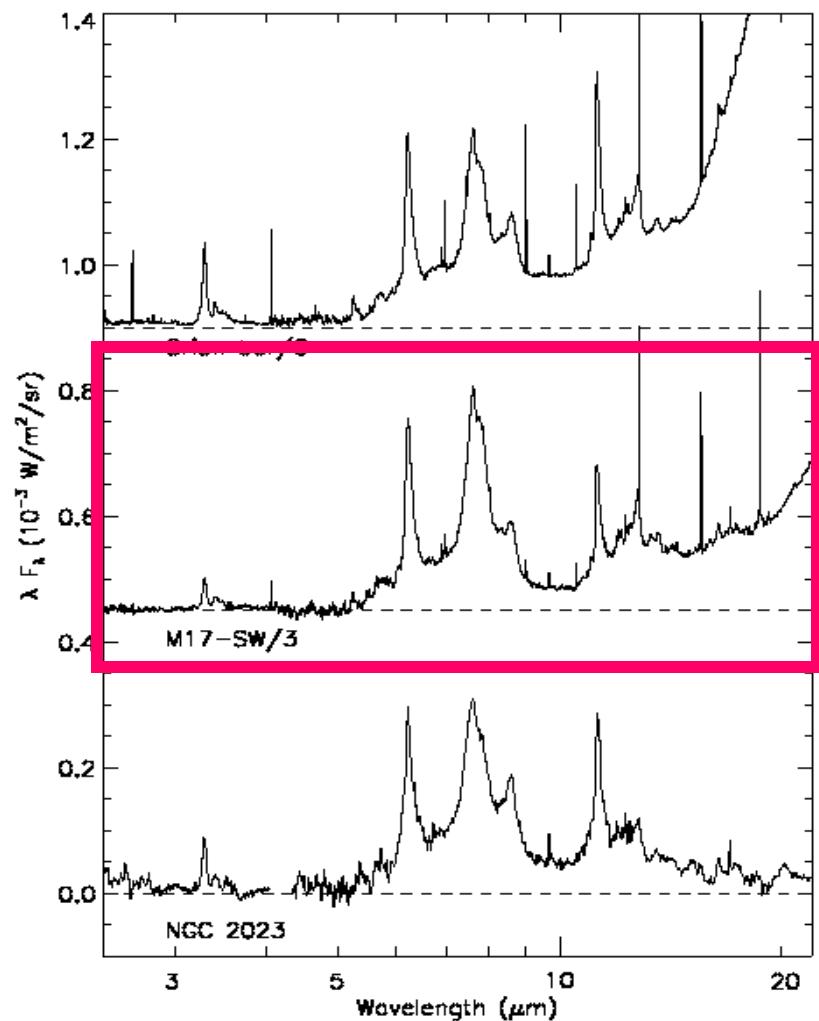
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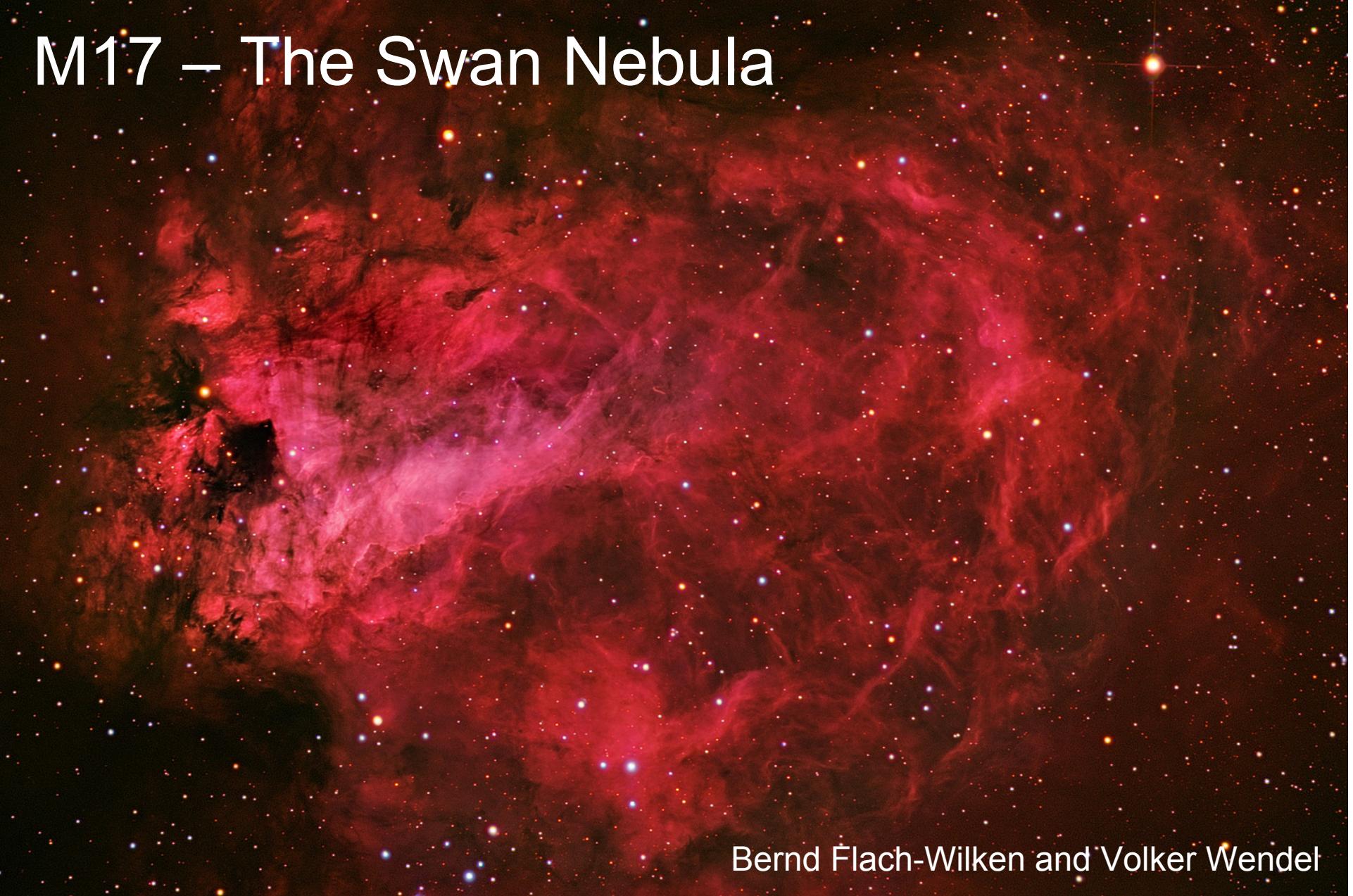


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# M17 – The Swan Nebula



Bernd Flach-Wilken and Volker Wendel

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M17



HST

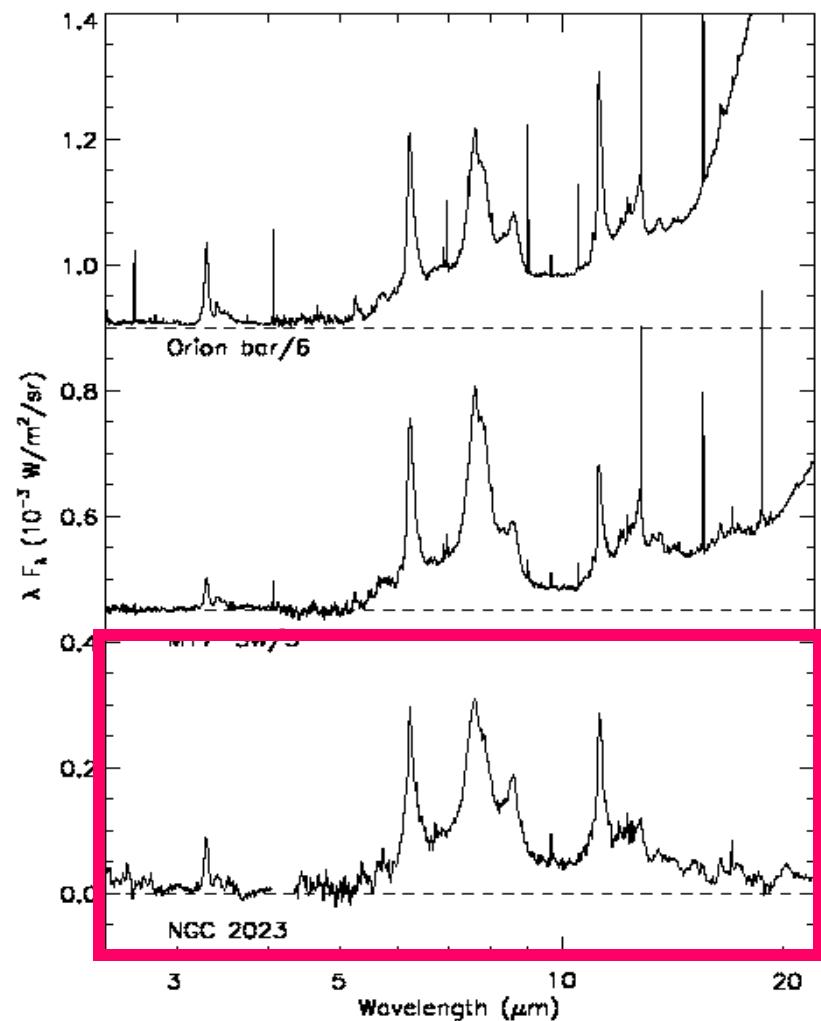
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# NGC 2023

Russell Croman

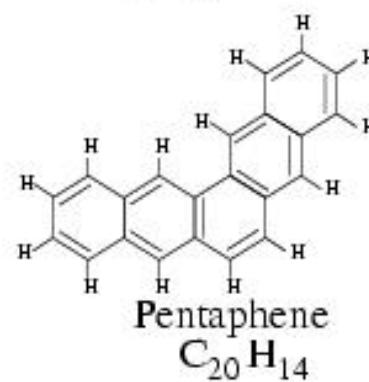
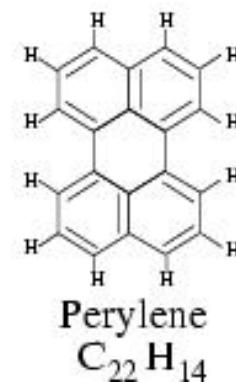
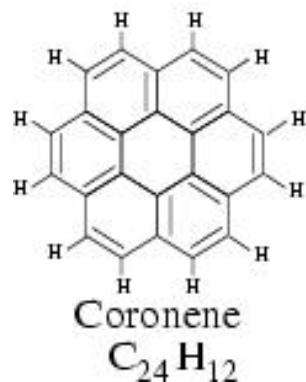
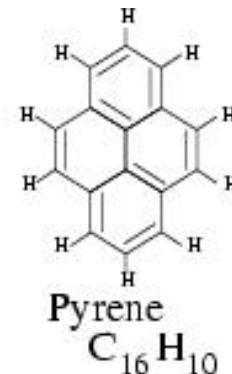
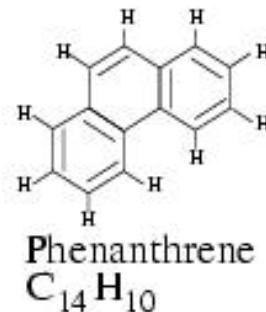
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# PAHs: Sources of the UIR Emission

## Polycyclic Aromatic Hydrocarbons



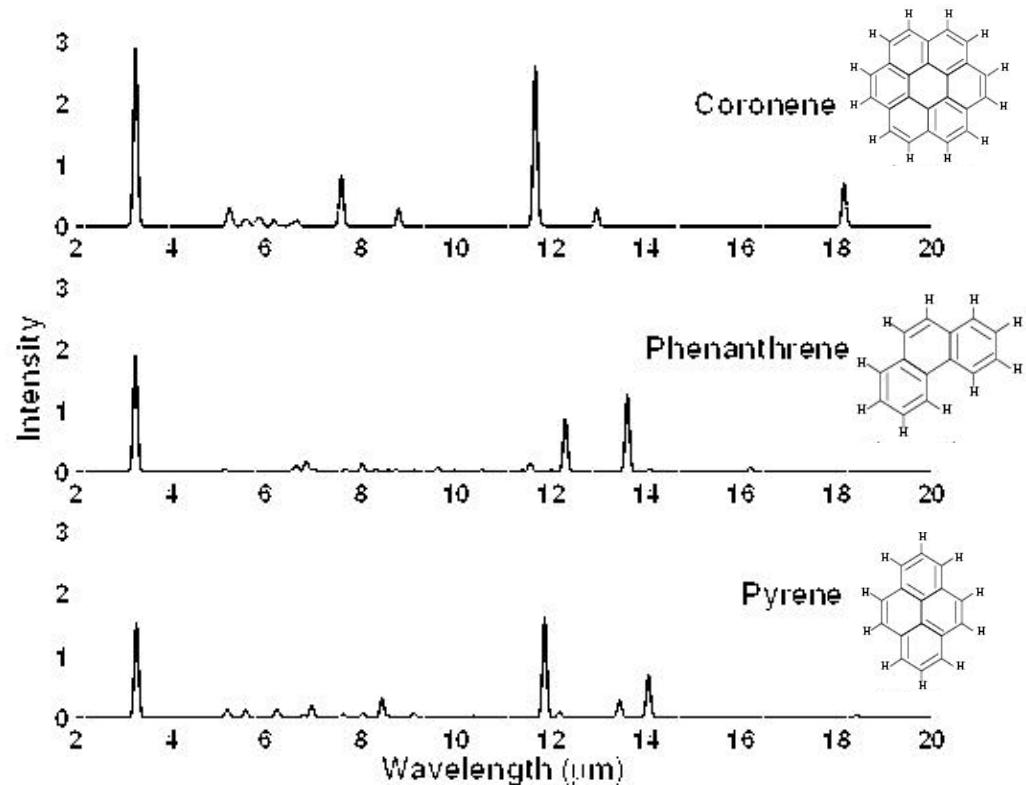
- Molecular bands near correct wavelengths
- Reasonable physical model for UV-driven IR emission

# Every PAH is an Individual

Spectra for ~1000 PAH species known from lab or theoretical work

- neutral, ions, and D, N, Fe, Mg-substituted

Each PAH has unique spectral features



# Why are PAHs so Interesting?

10-20% of all carbon atoms in the Interstellar Medium (ISM) are in PAH molecules

For this reason, PAH emissions are found in almost every cosmic environment in which there are concentrations of dust illuminated by ultraviolet radiation

They could be used to characterize the conditions of the ISM, and could be used as a tracer of star formation in the Milky Way

PAHs now appear to be important molecules on the pathway to life

# The PAH Identification Problem

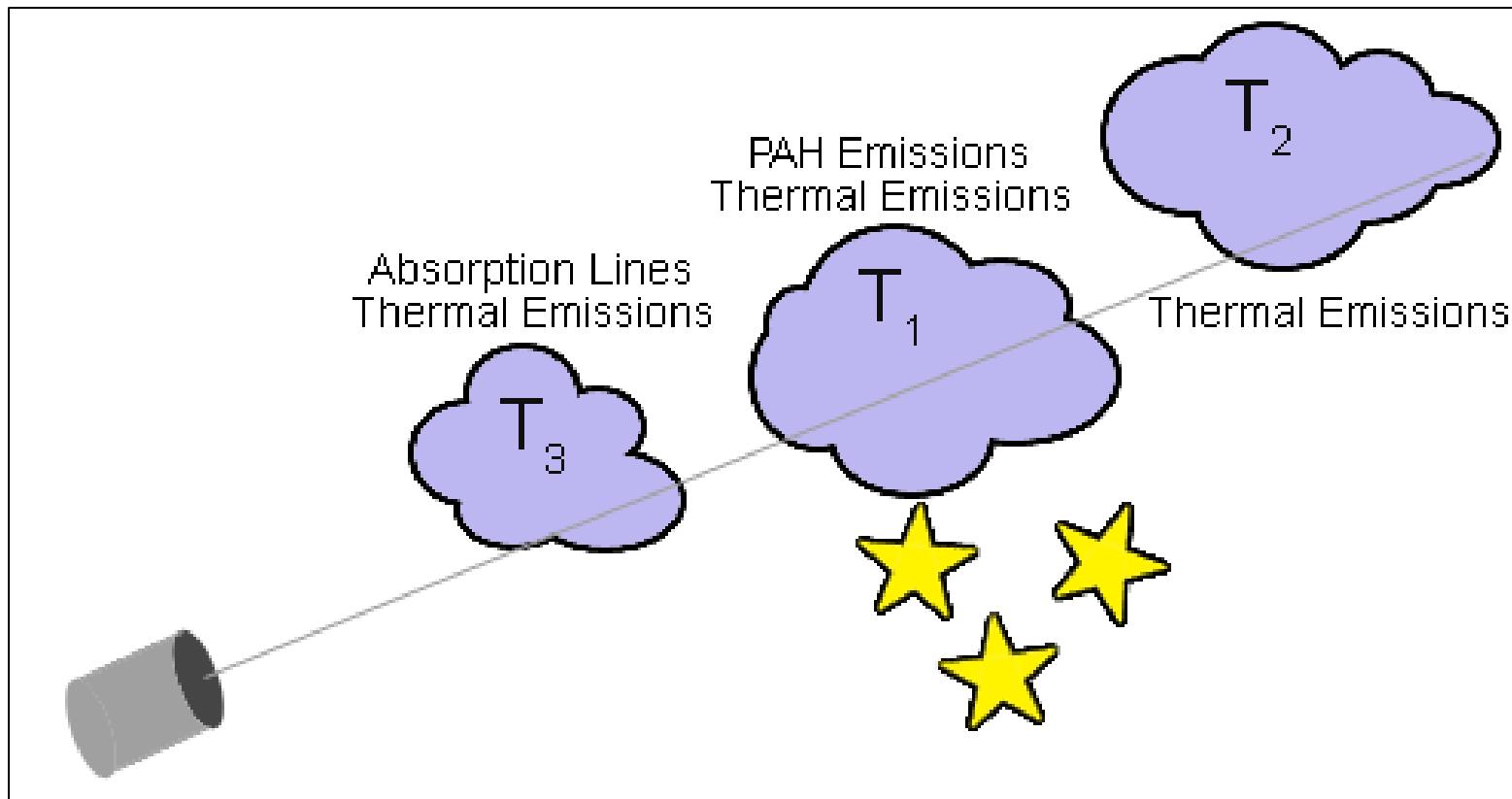
No astrophysical source shows the unique signature of any identifiable known PAH

Astrophysical sources appear to have:

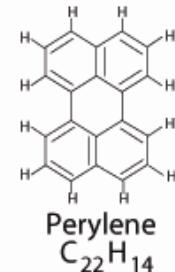
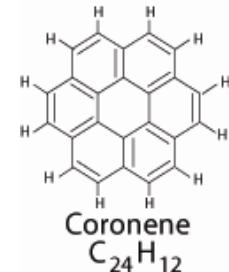
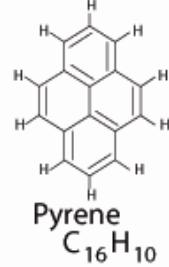
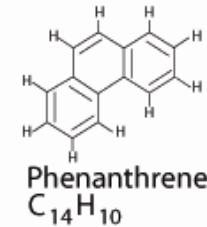
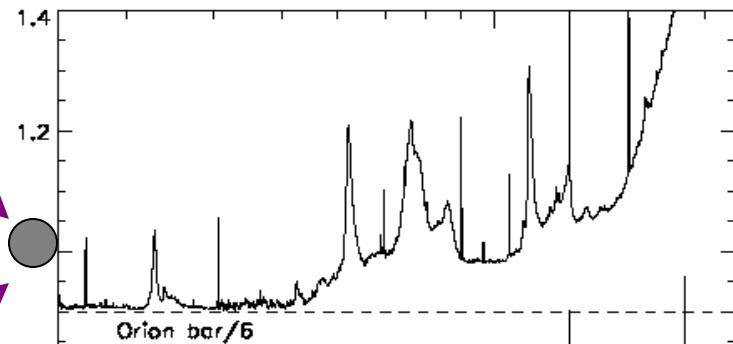
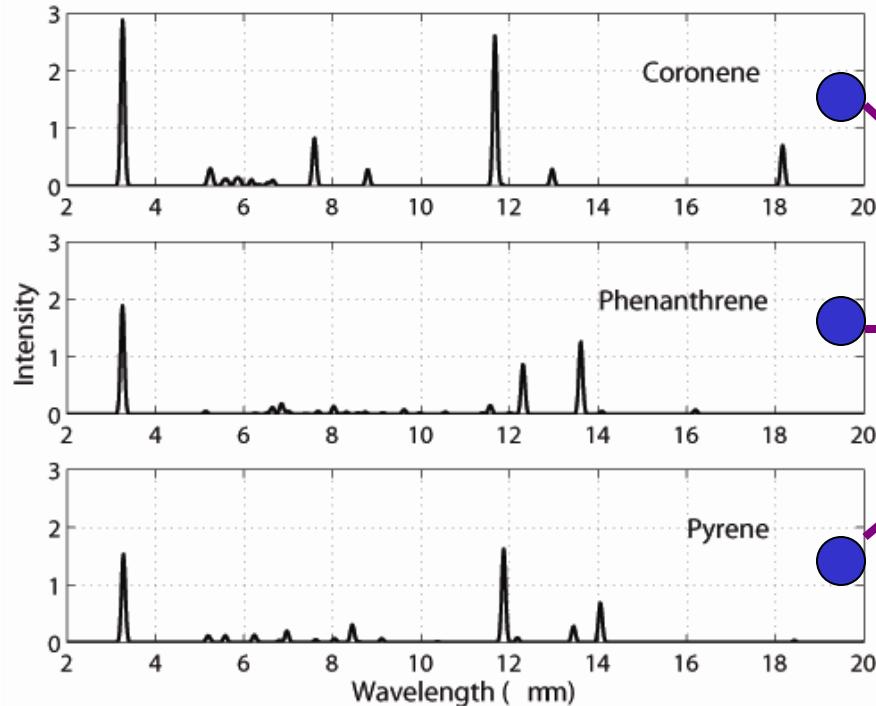
- multiple PAH species present
- different PAH-species concentrations depending on:
  - UV-intensity, temperature, and composition

# Modeling IR Spectra of Interstellar Clouds

# Complex IR Spectra



# Numerous PAH Species



Any number of thousands of PAH species can contribute to an observed spectrum.

# Modeling Important Features

$$F(\lambda) = \sum_{p=1}^P c_p \delta_p PAH_p(\lambda) + \sum_{k=1}^K A_k Planck(\lambda; T_k) + \sum_{g=1}^G A_g N(\lambda; \bar{\lambda}_g, \sigma_g)$$



PAH contributions

$c_p$  – PAH concentration

$\delta_p$  – PAH presence (YES or NO)

# Modeling Important Features

$$F(\lambda) = \sum_{p=1}^P c_p \delta_p PAH_p(\lambda) + \sum_{k=1}^K A_k Planck(\lambda; T_k) + \sum_{g=1}^G A_g N(\lambda; \bar{\lambda}_g, \sigma_g)$$



Planck Blackbody Radiators

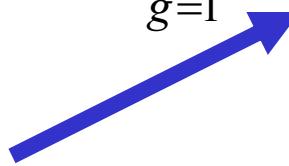
$A_k$  – Planck Amplitude

$T_k$  – Planck Temperature

$$Planck(\lambda; T_k) = \sqrt{\frac{\lambda_{\max}}{\lambda}} \frac{\exp(hc / \lambda_{\max} kT) - 1}{\exp(hc / \lambda kT) - 1}$$

# Modeling Important Features

$$F(\lambda) = \sum_{p=1}^P c_p \delta_p PAH_p(\lambda) + \sum_{k=1}^K A_k Planck(\lambda; T_k) + \sum_{g=1}^G A_g N(\lambda; \bar{\lambda}_g, \sigma_g)$$



Mixture of Gaussians

$A_g$  – Gaussian Amplitude

$\bar{\lambda}_g$  – Gaussian Mean

$\sigma_g$  – Gaussian Mean

# Modeling Important Features

$$F(\lambda) = \sum_{p=1}^P c_p \delta_p PAH_p(\lambda) + \sum_{k=1}^K A_k Planck(\lambda; T_k) + \sum_{g=1}^G A_g N(\lambda; \bar{\lambda}_g, \sigma_g)$$

1. PAH contributions (and atomic and ionic transitions)
2. Planck Radiators
3. Mixture of Gaussians

These three models describe the spectrum to first order.

# PAHs Pose Unique Difficulties

Most source separation problems consist of multiple mixtures and a handful of unknown sources with unknown contributions.

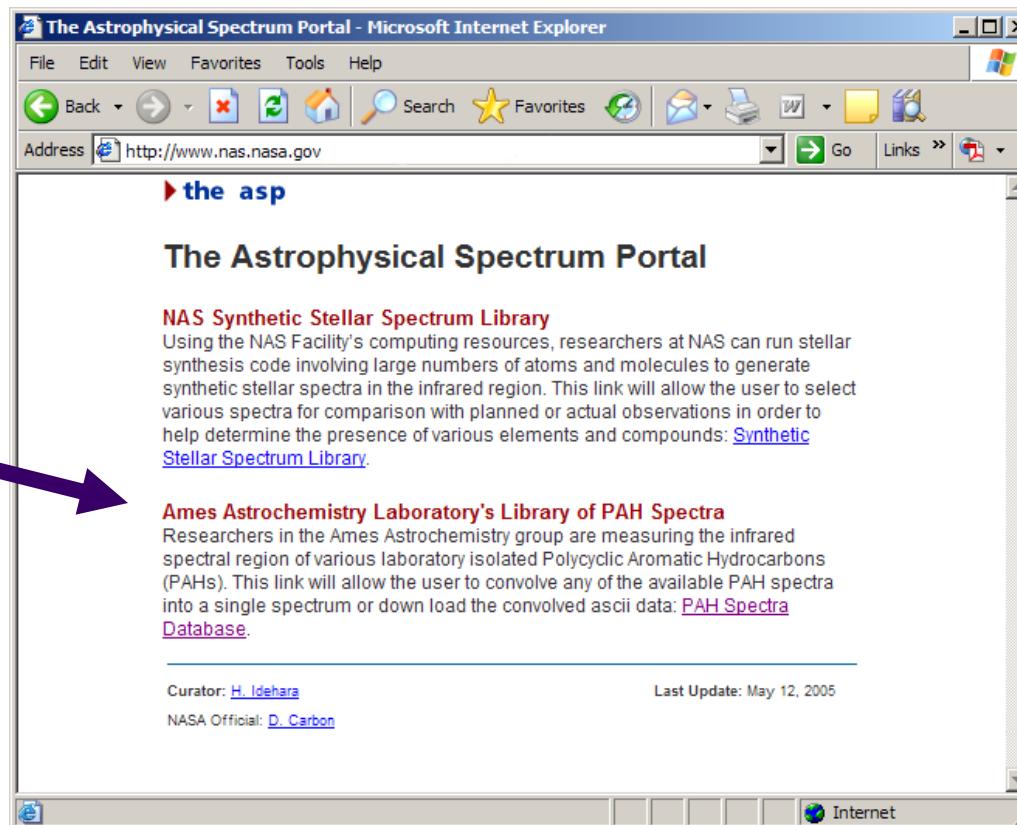
PAH spectral source separation consists of one mixture and numerous known sources with unknown contributions (and even some unknown sources).

There are potentially 100s to 1000s of species present.

- How do we tell which ones?
- How do we deal with the large number of spectra?

# Astrophysical Spectrum Portal

The PAH spectra database at NASA Ames Research Center will contain ~1000 PAH spectra



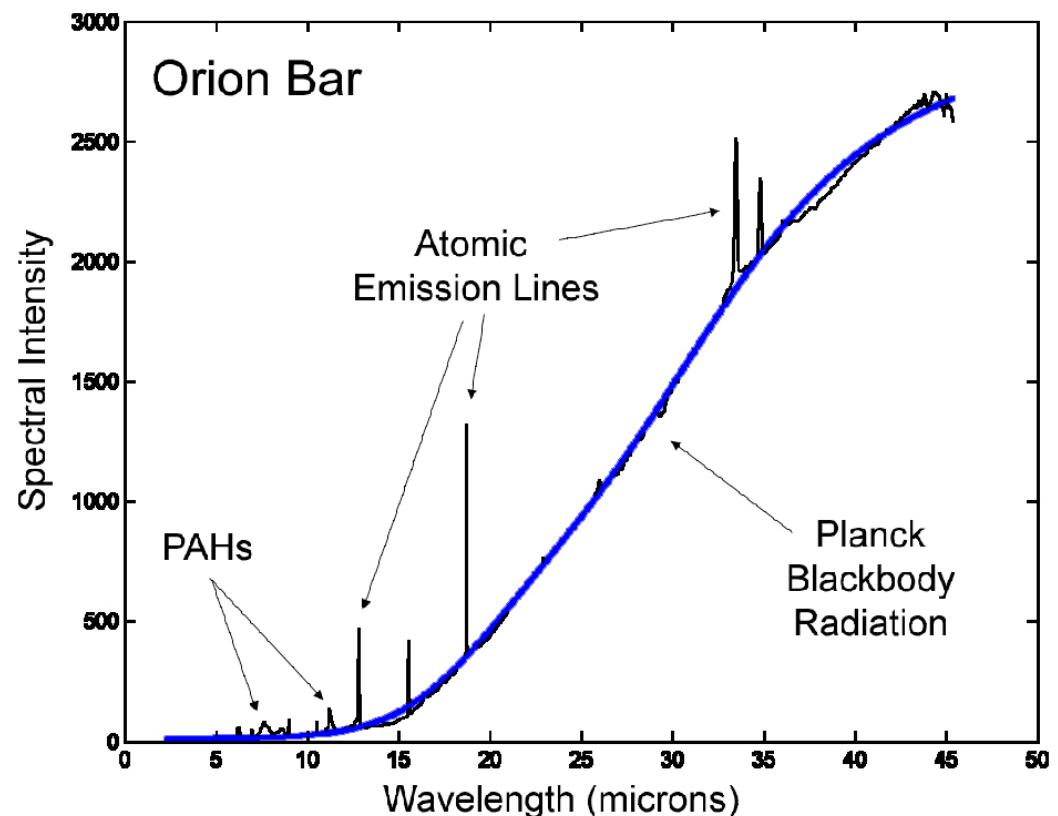
# Estimating Planck Backgrounds

# Estimating Planck Blackbodies

This figure shows a spectrum taken from the Orion Bar

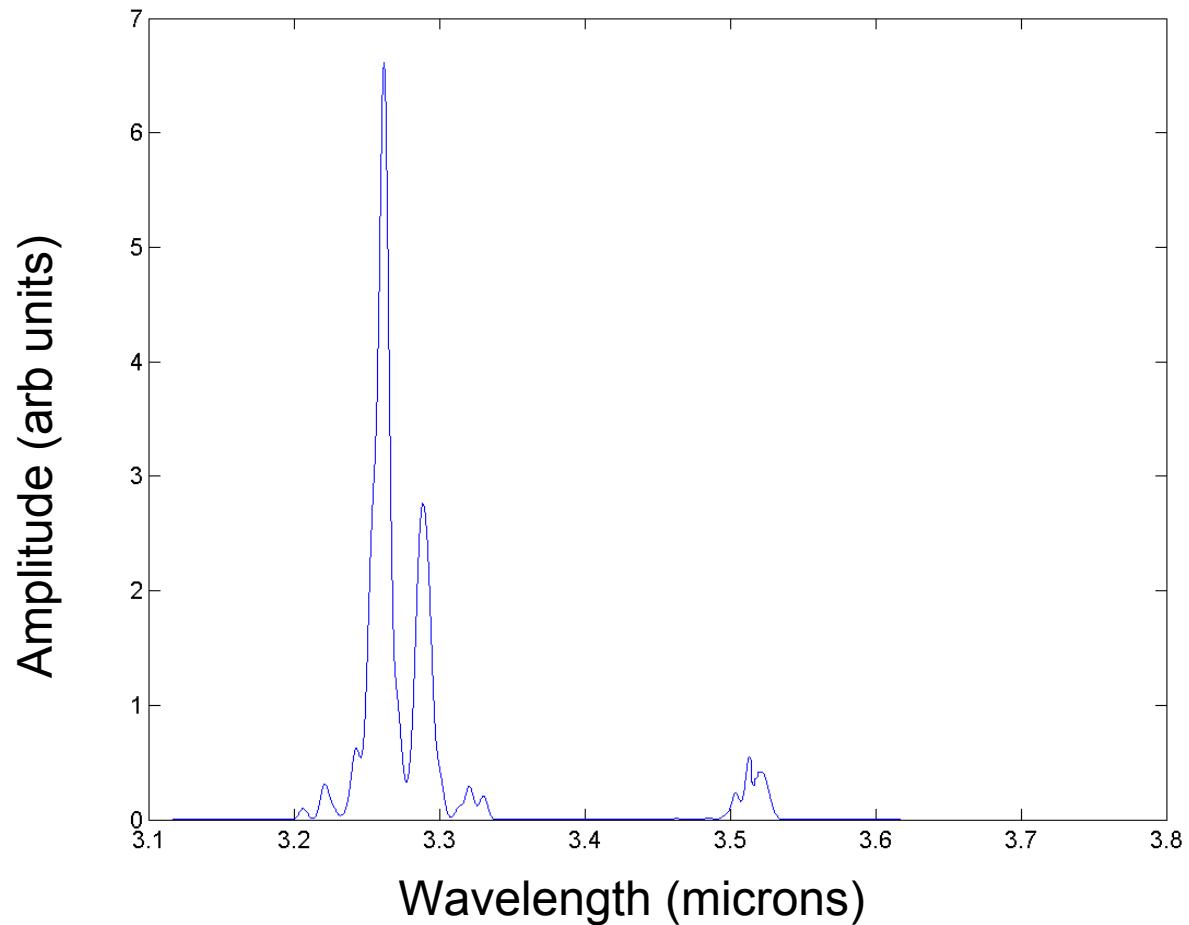
The black curve is the original data, the blue curve is the background estimation.

One blackbody radiator is at a temperature of  $61.043 \pm 0.004$  K, and there is possibly a second (36.3% chance), at a temperature around 18.8 K.

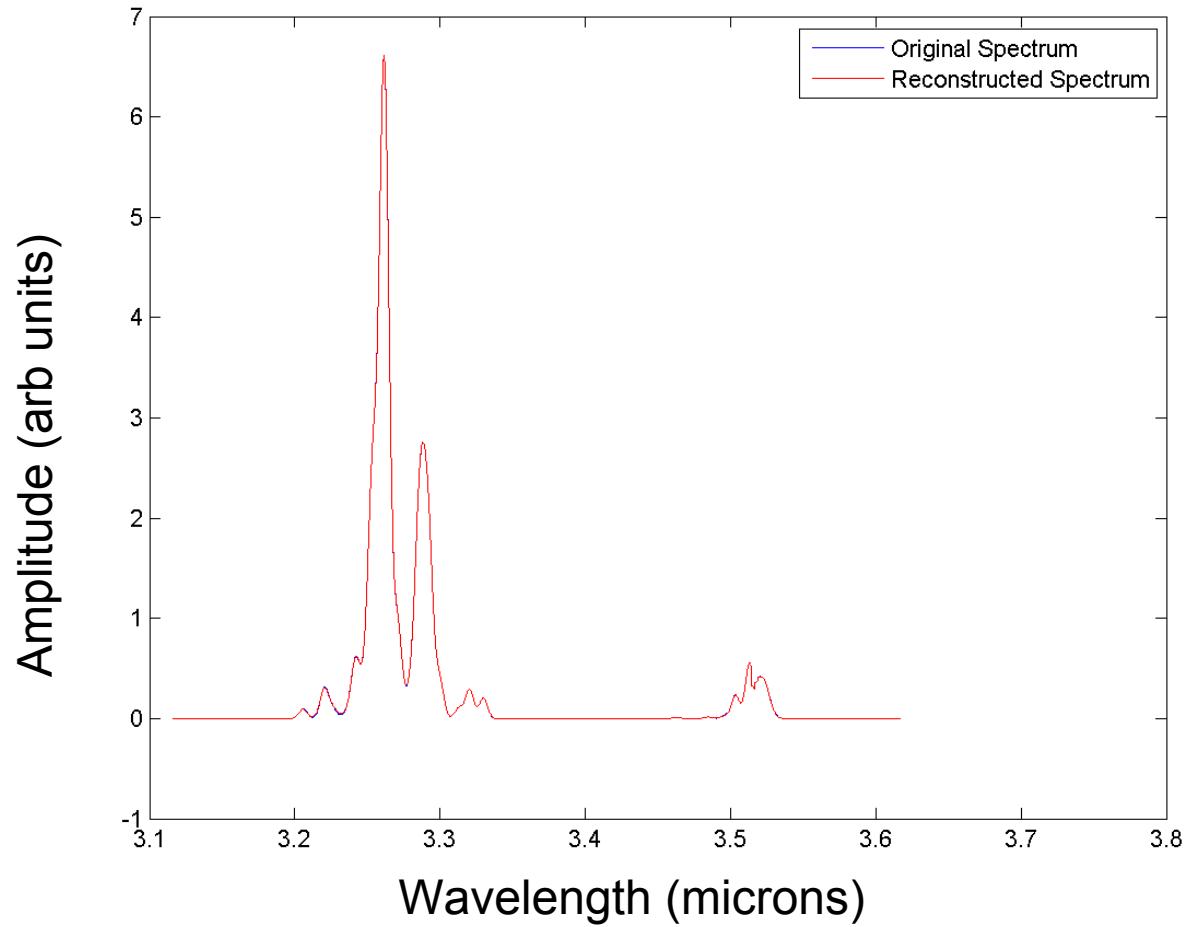


# Estimating PAHs

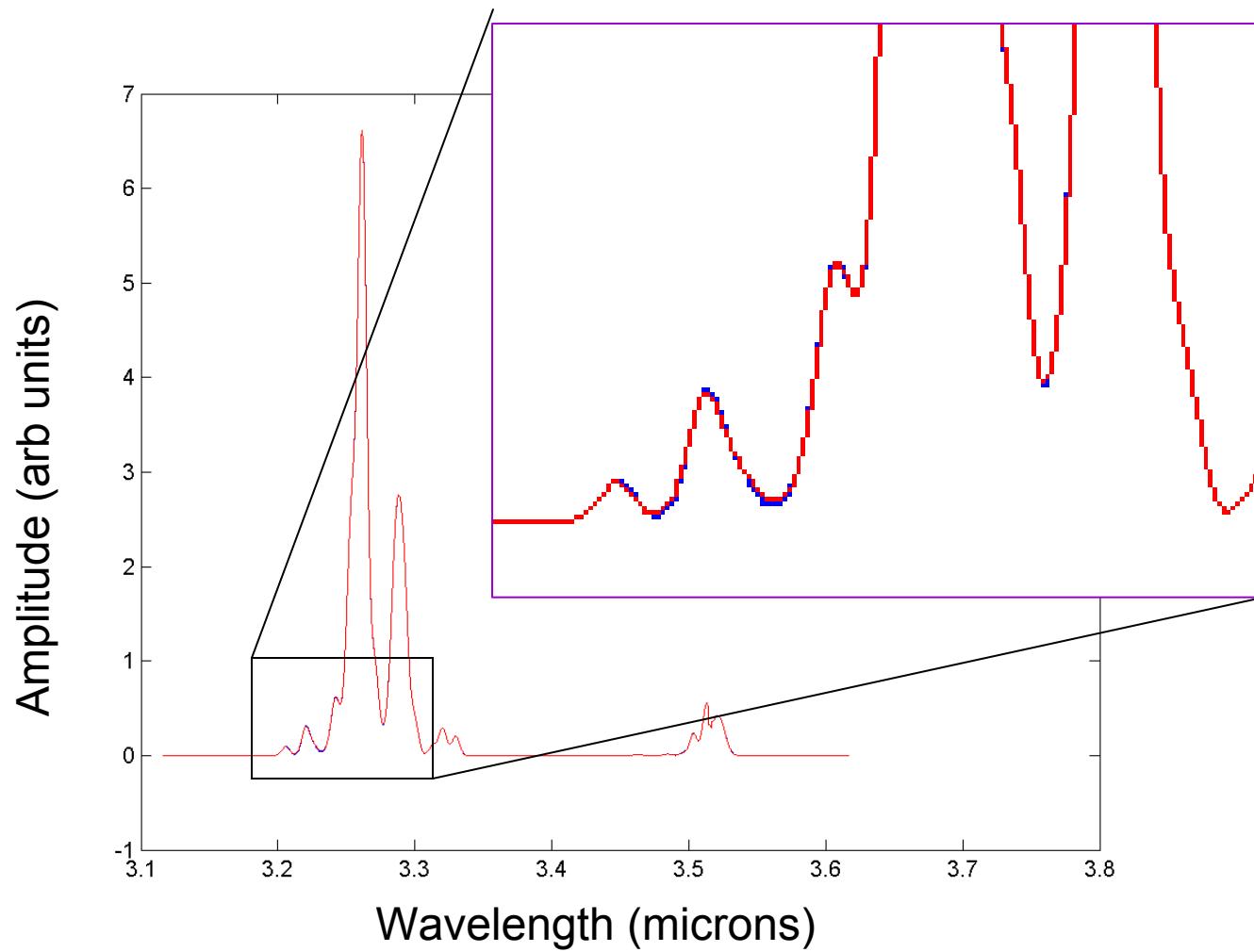
# Synthetic Mixture of 25 PAHs



# Reconstructed Estimate



# Reconstructed Estimate



# PAH Presence

Presence indicated by 0 or 1

Filed Circles

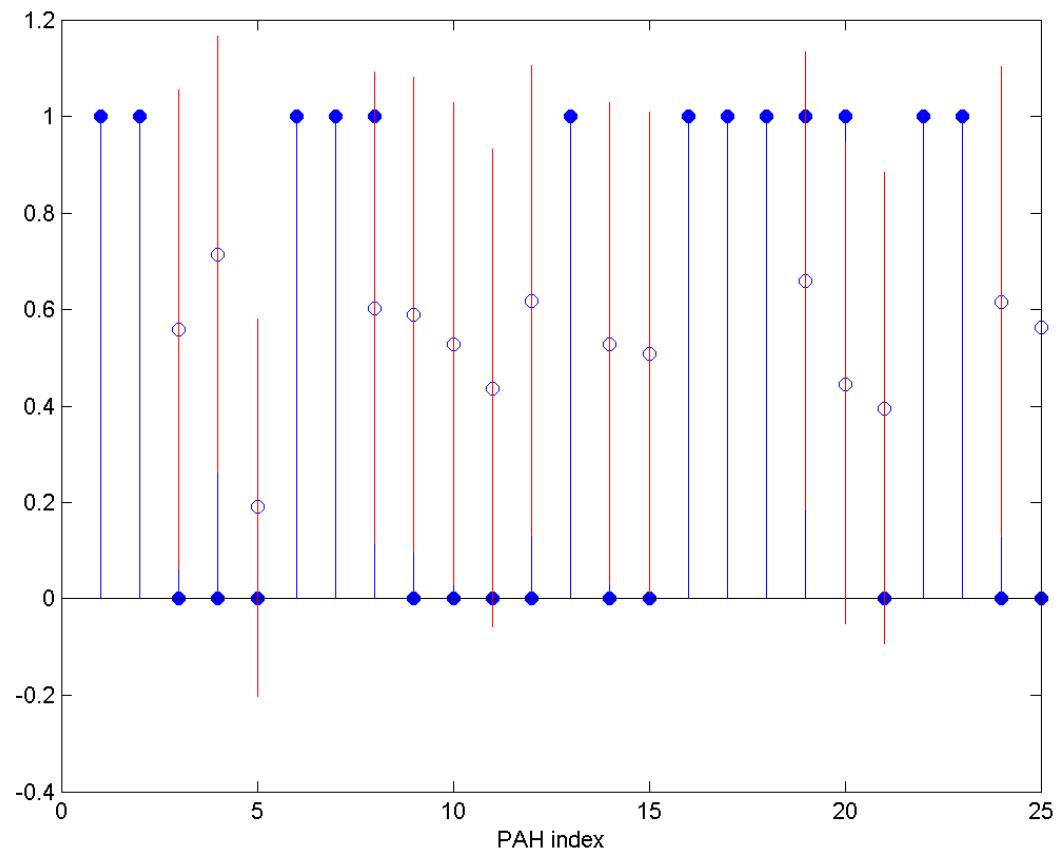
True Values

Hollow Circles

Est. Probability  
of Presence

Red Lines

Uncertainty in  
Presence  
Estimate



# PAH Concentrations

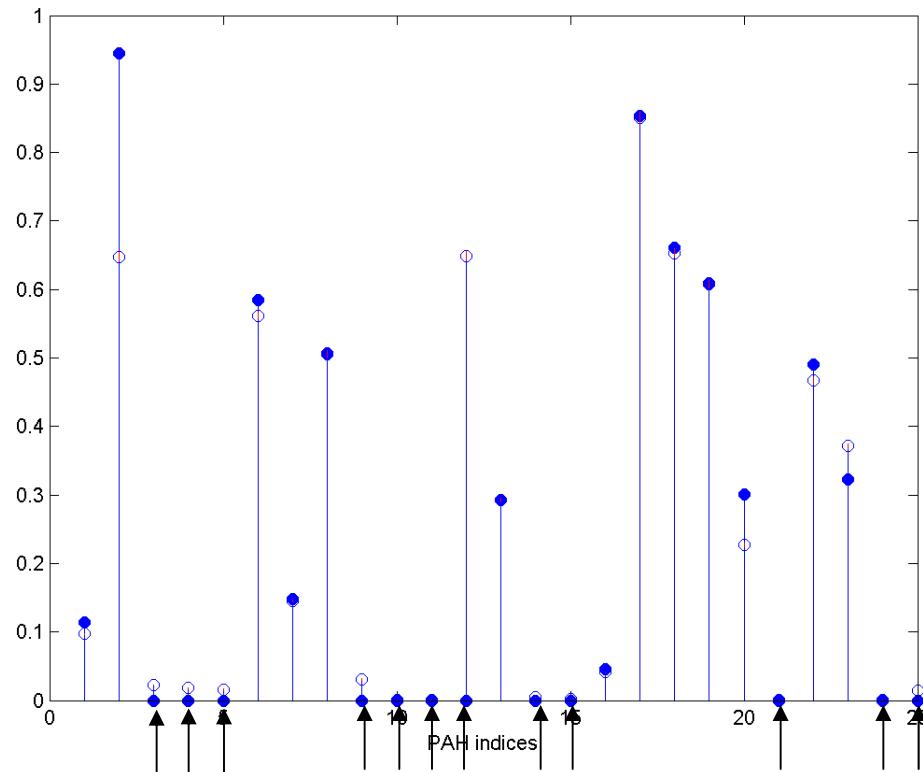
Concentration scaled from 0 to 1

Filed Circles  
True Values

Hollow Circles  
Est. Concentrations

Red Lines  
Uncertainty in  
Concentration Est.

Arrows indicate PAHs  
which are NOT PRESENT



# The Coming Year

# Future Work

The models are complex and estimation is time-consuming. We are investigating ways to speed this up by estimating background separately from PAHs, or to break the spectrum up into bands where the number of PAH contributions is minimal.

Continuing work with synthetic mixtures

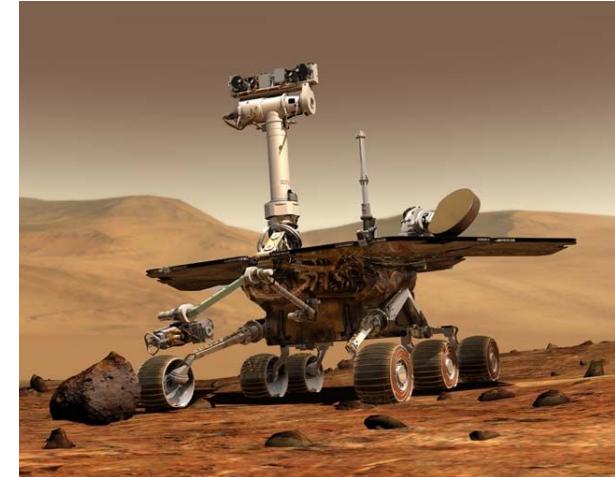
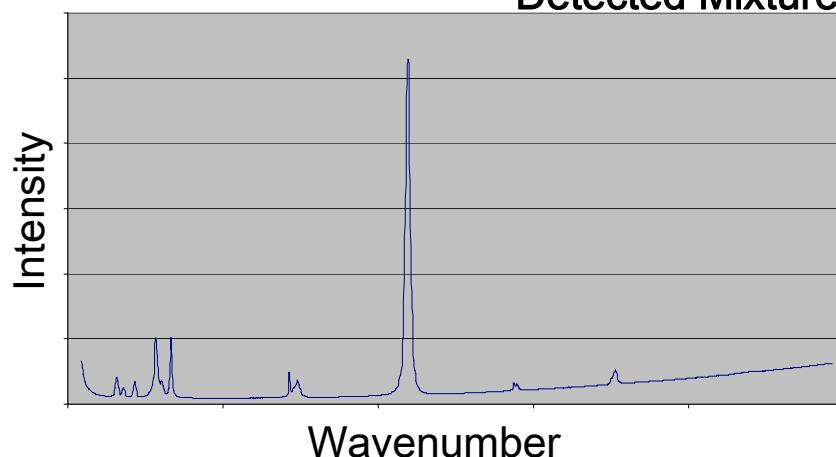
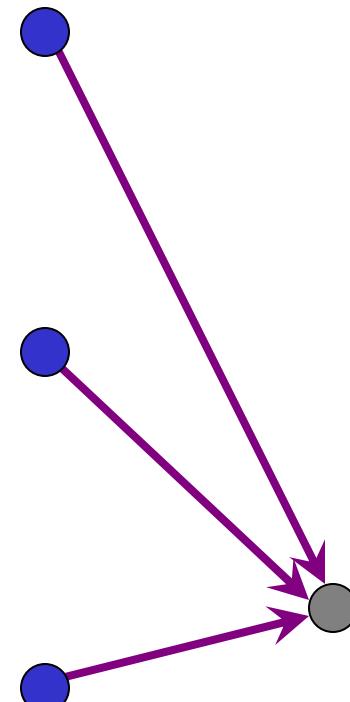
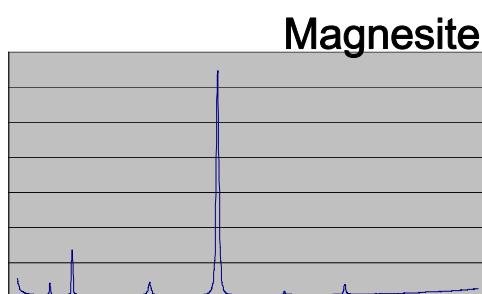
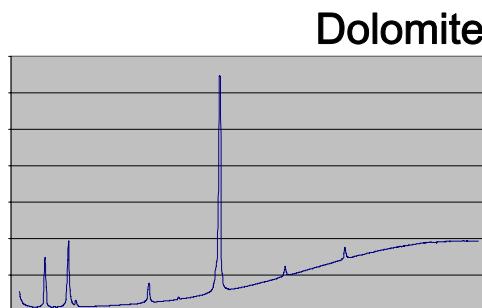
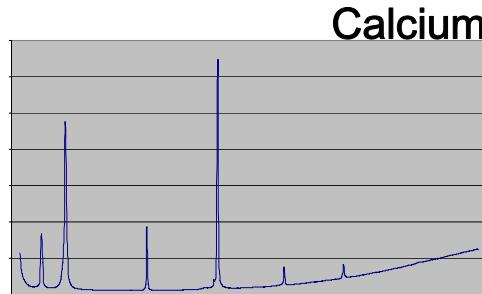
Moving to Real Data

Porting our algorithms to our Beowulf Cluster

Classifying PAHs based on structure, and estimating presence of classes rather than individuals

# Other Applications

# Mineralogy



Data from: Mary Garland, University of Toronto  
Raman Spectrum Excitation: 514 nm argon ion laser.  
<http://minerals.gps.caltech.edu/files/raman/toronto/toronto.htm>

# Stellar Composition

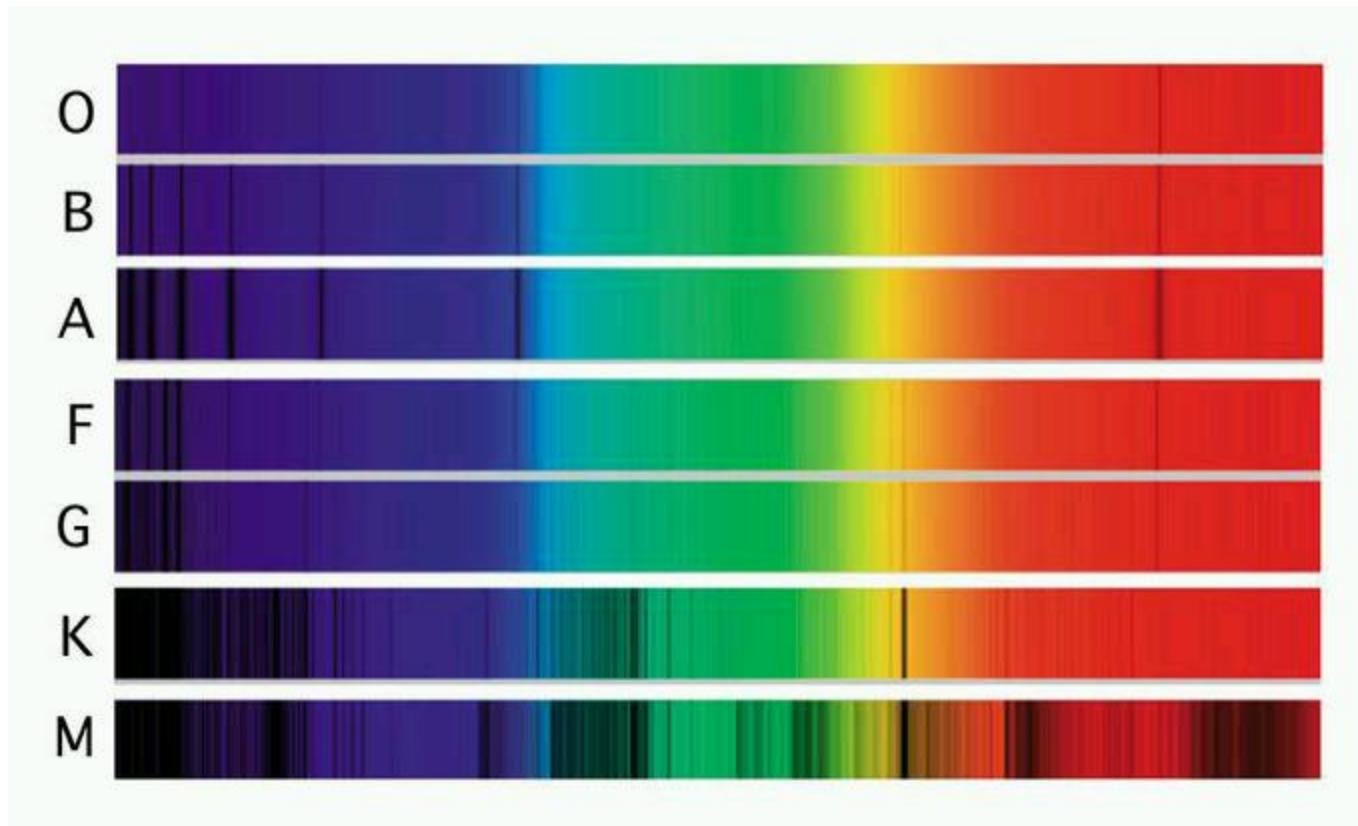
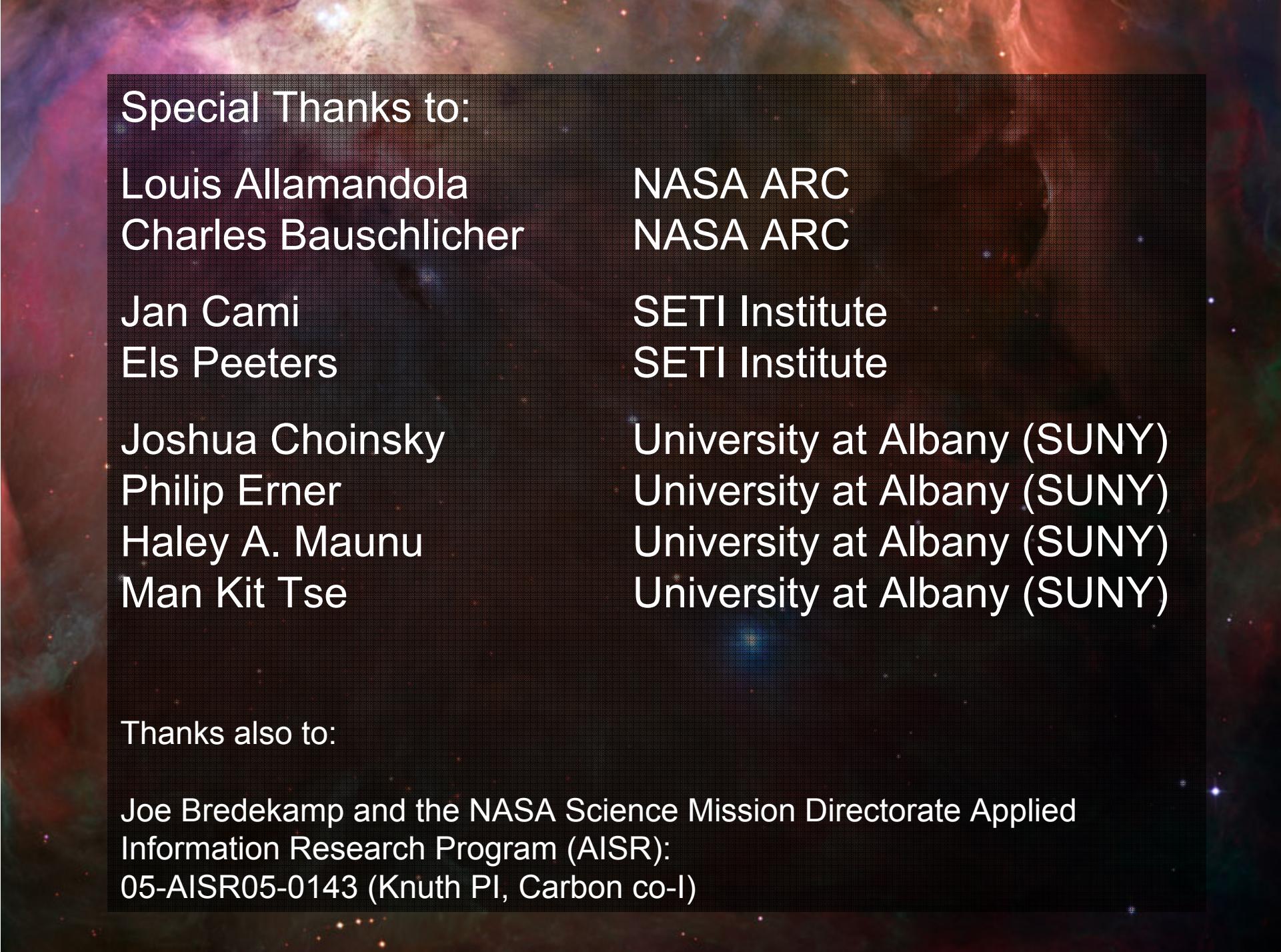


Image from Hanes, Queen's University

[http://www.astro.queensu.ca/~hanes/PHYS015-2007/Notes/DAH\\_Figs/Stellar\\_Spectra.jpg](http://www.astro.queensu.ca/~hanes/PHYS015-2007/Notes/DAH_Figs/Stellar_Spectra.jpg)



## Special Thanks to:

Louis Allamandola

Charles Bauschlicher

Jan Cami

Els Peeters

Joshua Choinsky

Philip Erner

Haley A. Maunu

Man Kit Tse

NASA ARC

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SETI Institute

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University at Albany (SUNY)

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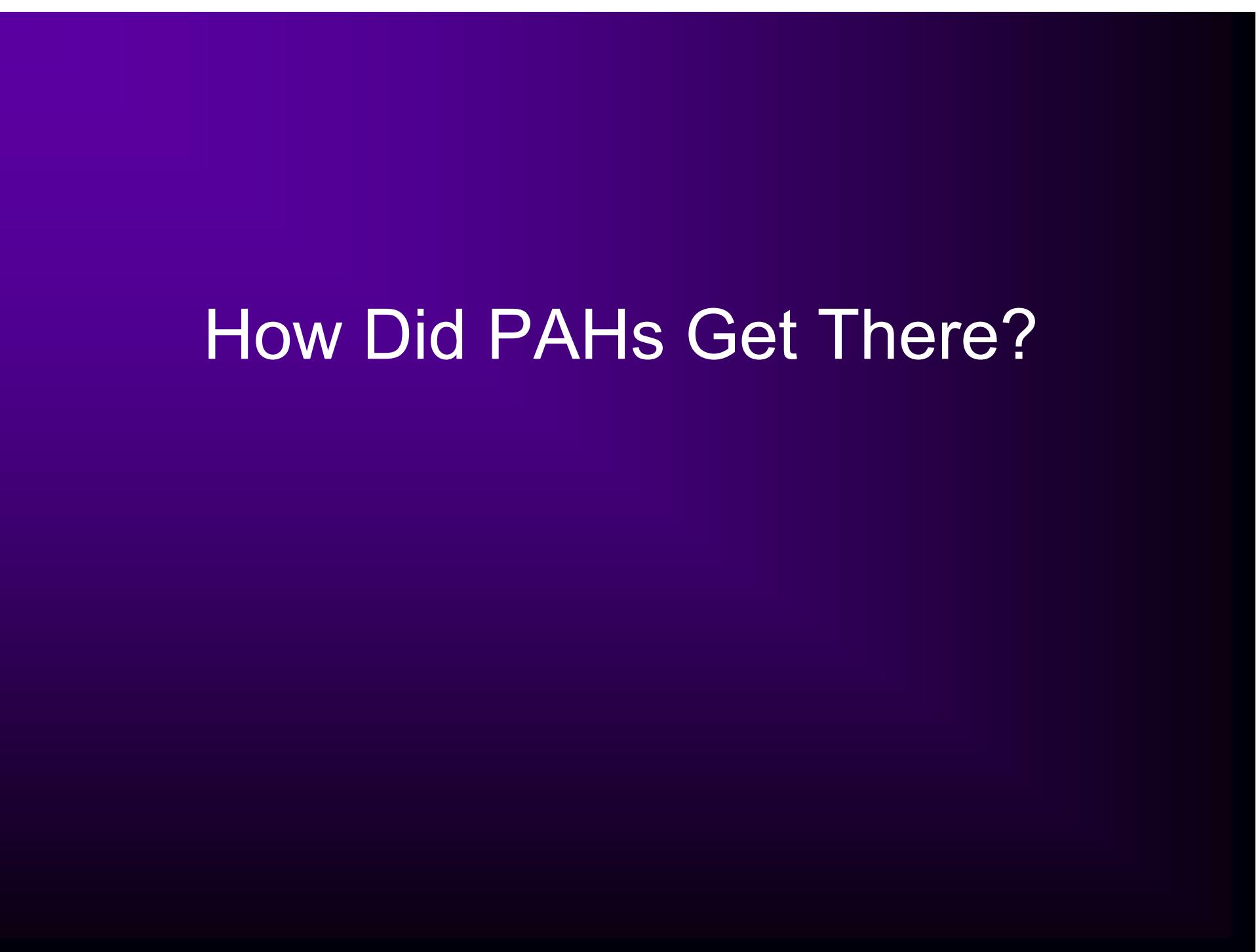
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## Thanks also to:

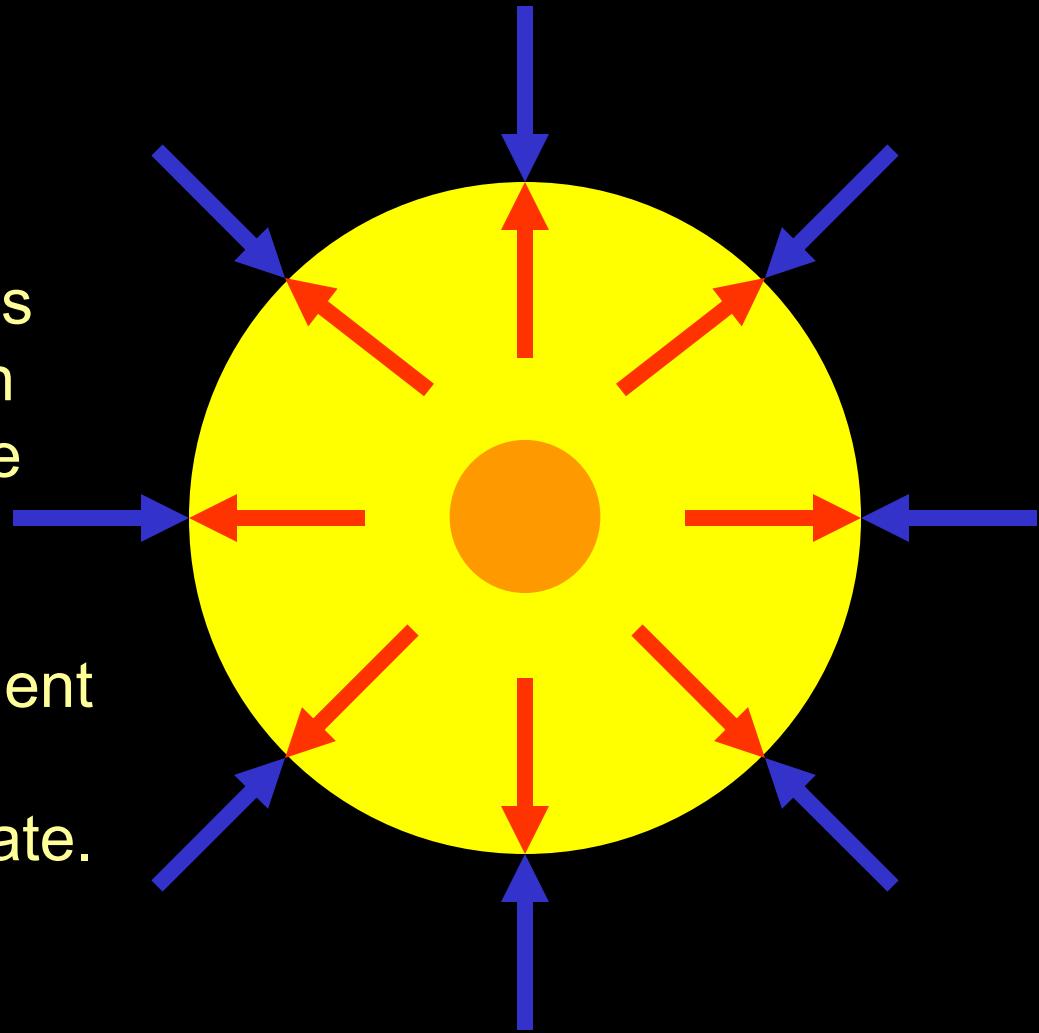
Joe Bredekamp and the NASA Science Mission Directorate Applied Information Research Program (AISR):  
05-AISR05-0143 (Knuth PI, Carbon co-I)

# How Did PAHs Get There?



# Forces Governing Stellar Structure

Nuclear fusion occurs in the high temperature and density present in the **core** and generates **thermal pressure**, which acts against the attractive **gravitational forces**.



As long as there is sufficient fuel in the core, the star remains in this steady-state.

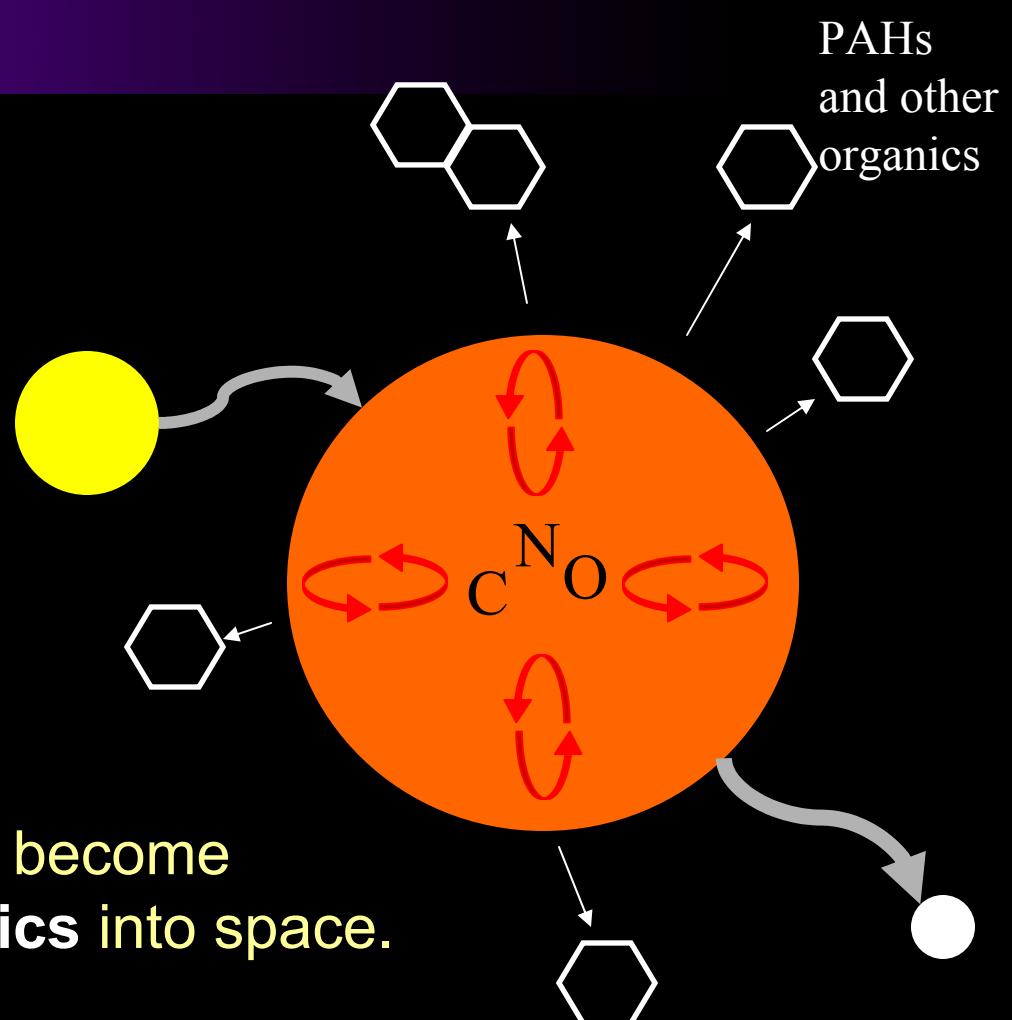
# Stellar Evolution

Stars eventually run out of Hydrogen to fuse, and begin to collapse cramming more matter into the core.

The greater densities and pressures allow creation of C N and O.

The star swells and cools to become a **Red Giant** spewing **organics** into space.

When fuel finally runs out, the star collapses into a **hot** White Dwarf



# Why are PAHs so Interesting?

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For this reason, PAH emissions are found in almost every cosmic environment in which there are concentrations of dust illuminated by ultraviolet radiation

They could be used to characterize the conditions of the ISM, and could be used as a tracer of star formation in the Milky Way

PAHs now appear to be important molecules on the pathway to life

# Non-Negative Least Squares

**Minimize:**  $\chi^2$

**Subject to:**  $c_i > 0$

$$\chi^2 = \sum_{l=1}^L (F_{\text{obs}}(\lambda_l) - F_{\text{mod}}(\lambda_l))^2$$

$$\chi^2 = \sum_{l=1}^L \left( F_{\text{obs}}(\lambda_l) - \sum_i c_i s_i(\lambda_l) \right)^2$$

Estimate PAH contributions

Works alright, but with only small numbers of PAHs and with little spectral overlap.